

# Macromolecules

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## Supplementary tables

**Table S-I.** Fractional coordinates of the Lovinger structure III<sub>au</sub> obtained by optimization, using MSXX. The cell is orthorhombic with  $a = 9.68 \text{ \AA}$ ,  $b = 4.98 \text{ \AA}$ , and  $c = 9.13 \text{ \AA}$ . The space group is  $Pca2_1(C_{2v}^5)$ .

Atom	X	Y	Z
C <sub>1</sub>	0.248	0.730	0.917
C <sub>2</sub>	0.370	0.818	0.825
C <sub>3</sub>	0.368	0.718	0.667
C <sub>4</sub>	0.242	0.802	0.579
F <sub>1</sub>	0.491	0.732	0.886
F <sub>2</sub>	0.382	0.090	0.827
F <sub>3</sub>	0.128	0.681	0.637
F <sub>4</sub>	0.218	0.069	0.596
H <sub>1</sub>	0.155	0.824	0.877
H <sub>2</sub>	0.236	0.515	0.908
H <sub>3</sub>	0.461	0.796	0.616
H <sub>4</sub>	0.375	0.502	0.666

**Table S-II.** Piezoelectric constants  $g_{ij}$  (C/m<sup>2</sup>) calculated at the experimental structures (except for form III<sub>au</sub>, where the optimized structure is used).

MSXX						MSXXS					
Form I <sub>p</sub>											
0.0	0.0	0.0	0.0	-0.15	0.0	0.0	0.0	0.0	0.0	-0.15	0.0
0.0	0.0	0.0	-0.024	0.0	0.0	0.0	0.0	0.0	-0.067	0.0	0.0
-0.007	-0.01	-0.15	0.0	0.0	0.0	0.087	-0.073	-0.22	0.0	0.0	0.0
Form III <sub>pu</sub>											
0.057	0.059	-0.19	0.0	-0.004	0.0	0.12	0.062	-0.26	0.0	-0.006	0.0
0.0	0.0	0.0	0.007	0.0	0.048	0.0	0.0	0.0	0.031	0.0	0.034
0.017	-0.017	0.18	0.0	0.071	0.0	0.032	0.0036	0.19	0.0	0.074	0.0
Form II <sub>pd</sub>											
0.0	0.0	0.0	0.0	0.067	0.0	0.0	0.0	0.0	0.0	0.069	0.0
0.0	0.0	0.0	0.045	0.0	0.0	0.0	0.0	0.0	0.032	0.0	0.0
-0.21	0.030	0.023	0.0	0.0	0.0	-0.27	0.028	0.089	0.0	0.0	0.0
Form III <sub>au</sub>											
0.0	0.0	0.0	0.0	-0.0002	0.0	0.0	0.0	0.0	0.0	0.024	0.0
0.0	0.0	0.0	0.0096	0.0	0.0	0.0	0.0	0.0	0.012	0.0	0.0
-0.026	0.024	0.18	0.0	0.0	0.0	-0.011	0.042	0.18	0.0	0.0	0.0

**Table S-III.** Elastic constants( $C_{IJ}$  in GPa) and piezoelectric moduli ( $d_{ij}$  in pC/N) of PVDF form I<sub>p</sub>.

	TKTF <sup>a</sup>	MSXXS	MSXX	Exper
$C_{11}$	23.60	23.7	25.5	
$C_{22}$	10.64	11.8	12.4	
$C_{33}$	238.24	266.8	283.4	
$C_{12}$	1.92	2.4	3.0	
$C_{13}$	3.98	4.7	4.0	
$C_{23}$	2.19	3.1	2.4	
$C_{44}$	4.40	3.7	3.5	
$C_{55}$	6.43	5.2	5.1	
$C_{66}$	2.15	4.0	4.0	
$d_{15}$	-30.70	-41.9	-41.3	
$d_{24}$	-4.28	-16.8	-5.9	-38.3 <sup>c</sup>
$d_{31}$	-0.25	0.57	0.07	
$d_{32}$	-4.05	-1.3	1.1	
$d_{33}$	-25.19	-18.8	-12.7	-20 $\pm$ 5 <sup>b</sup>

<sup>a</sup> Reference 23.<sup>b</sup> Reference 23.<sup>c</sup>Reference 26.